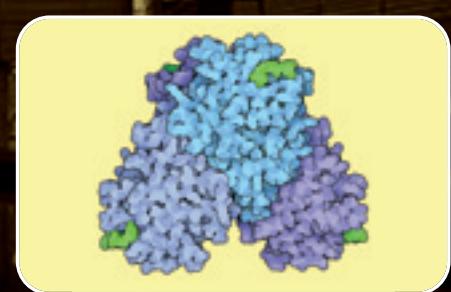
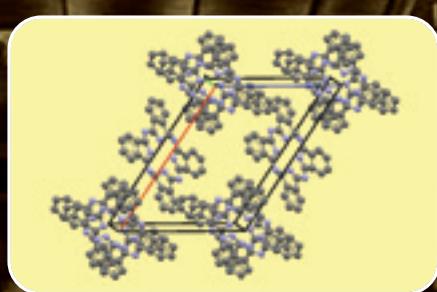


Crystallography News

British Crystallographic Association

Issue No. 136 March 2016

ISSI 1467-2790



Nottingham Business School awaits takeover by crystallographers

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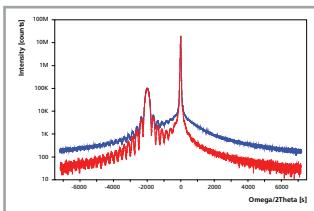
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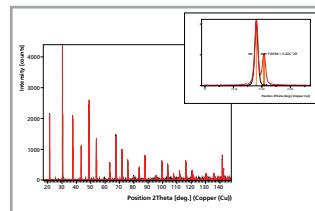
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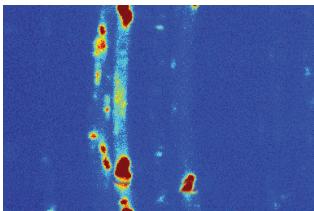
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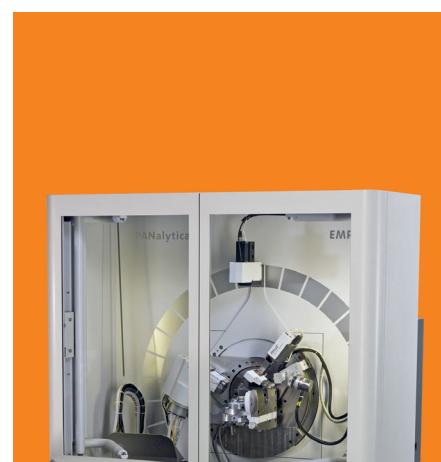
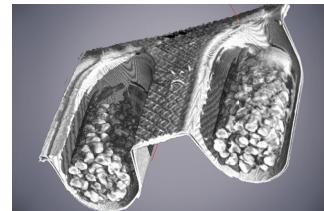
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2D



3D

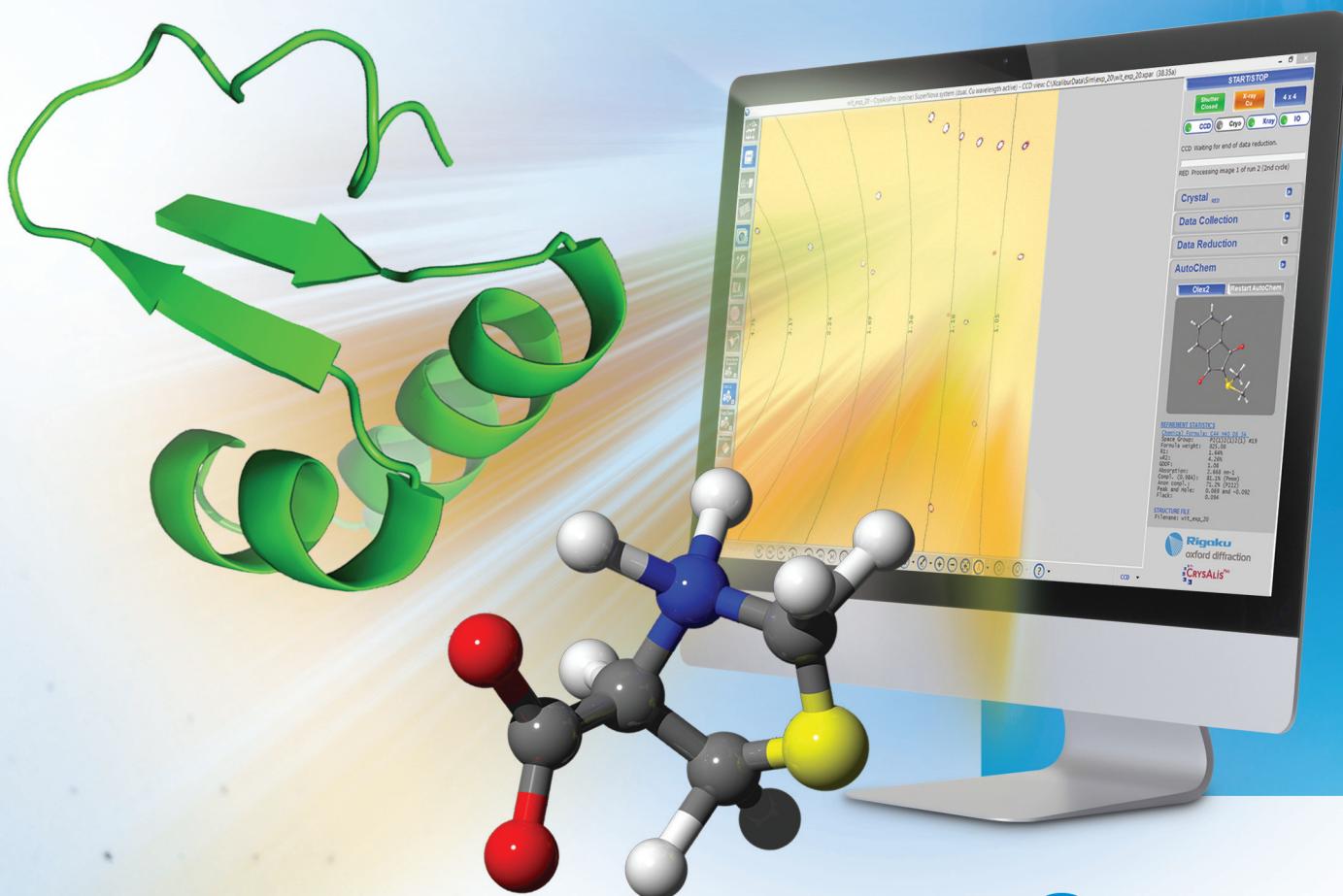


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These details are not divulged to any others without your permission. You may inspect your entry during the Annual Meeting, or otherwise by application to the BCA Administrative Office. We will be happy to amend entries at any time.

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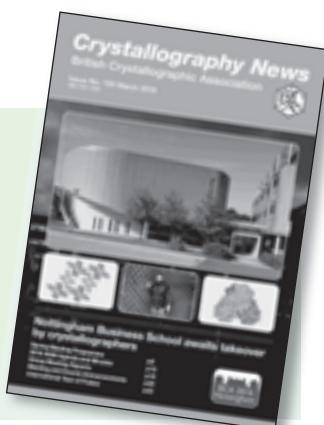
Crystallography News March 2016

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This month's cover:

Nottingham Business School,
phthalocyanine,
huge NaCl model (BBC News),
concanavalin A.



From the President



I AM writing this column having just returned from beam time at Diamond Light Source. I find it's always an exciting time to be there to do science that is simply not possible even in the best home laboratory. Like the ISIS facility alongside it, it is a facility that has an enormous impact on the UK crystallographic community and on a much broader community across all the sciences and engineering. It is exciting to see new developments there including the new macromolecular crystallography beamlines VMXm and VMXi under construction, the new pair-distribution function beamline (XPDF at I15-1) approaching the time of its first users, and the major upgrade to chemical crystallography capabilities at beamline I19, which was being put through its paces by its first users in January 2016.

This is my final column of the 2015-16 cycle and is a time to be looking forward to the upcoming BCA Spring Meeting in Nottingham. At the time of writing, the abstract deadline has just closed and an outstanding programme of speakers has been assembled, together with a strong showing of poster presentations and a full commercial exhibition. The main meeting will feature lectures from **Arwen Pearson**, who will give the **Lonsdale Lecture**, and **Christer Åkeröy**, who will give the **BCA Prize Lecture**. Wednesday afternoon will include the Early Career Awards Symposium, featuring lectures from the awardees of the BCA groups. Further details of the programme can be found on page 6 of the Newsletter and on the meeting website. The YCG satellite meeting, held directly prior to the main meeting, features an interesting session on **Forgotten Methods in Crystallography**.

Congratulations also to **Jonathan Brooks-Bartlett** who will deliver the **Parkin Lecture**, which is named in honour of the late Dr. Andrew Parkin and recognises outstanding contributions to promoting science, raising public awareness of science, teaching crystallography/science or showing originality in outreach and teaching activities. Jonny has been one of the star performers in outreach activities among BCA members in recent years. I am grateful to Programme Chair **Phil Lightfoot** and the whole Programme Committee for their commitment over the past year in putting the meeting programme together, and to our colleagues at Hg3 for smoothly handling the logistical side of the conference planning and delivery. The Annual General Meeting will be held during its usual Wednesday early evening slot and will see elections for the positions of Vice President, Secretary and one of the three Ordinary Member positions on Council. Earlier that day the AGMs for the BSG, CCG, IG and PCG groups will be held and will include committee member elections (AGM for the YCG is on the Monday).

At our recent BCA Officers Meeting, in addition to receiving updates on the 2016 Spring Meeting, we discussed planning for future meetings. It's never too early to start thinking ahead and I encourage members to send your suggestions for 2017 symposia topics to the BCA group representatives, who will be pleased to hear from you. I was able to announce in my previous column that we will be holding our 2017 Spring

Meeting at Lancaster University and can now confirm that we will be holding the 2018 meeting at Warwick University. We also spent some time discussing Education & Outreach Activities. **Simon Coles**, our E&OA Officer, has been developing plans to make the BCA more self-sufficient in its activities in this area as well as being able to continue to team up with other organisations. We will be looking for members to help to develop new outreach activities that can be delivered to schools, science fairs and public outreach events around the country. The BCA has been particularly active in its outreach in recent years and we hope to continue and build upon this success.

Finally, I am delighted to be able to announce the award of BCA Honorary Life Memberships to two highly respected and distinguished members of the UK crystallographic community. Honorary Life Membership is the BCA's highest membership accolade, awarded to a small and select band of colleagues who have contributed significantly to crystallographic science and to the work of the BCA. **Eleanor Dodson**, FRS has previously received the IUCr Ewald Medal, the ECA Perutz Prize and ACA Fankuchen Award for her research and teaching in crystallography and has played an active role in the BCA and its conferences over many years. **Olga Kennard**, FRS is recognised not only for her outstanding research contributions in crystallography but, in particular, for her role in founding the CCDC and leading the organisation for many years thereafter. She has also made valuable contributions to the BCA over a number of years, including as a Founding Member. A list of Honorary Life Members can be found on the BCA website.

I look forward to seeing many of you in Nottingham for what promises to be an excellent Spring Meeting.

Lee Brammer



BCA Council 2016

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(The dates in parentheses indicate the end of the term of office).

Full committee details on the BCA website www.crystallography.org.uk

From the Editor



AT this time the focus of our attention is on the upcoming BCA Spring Meeting. The updated information in this issue demonstrates that there will be abundant topics of interest to every kind of crystallographer. In addition, the central location of our venue, the University of Nottingham, makes it easy to get to from just about anywhere in

the UK. I just want to remind readers that the University of Nottingham seems to have taken as its motto those lines from Land of Hope and Glory "Wider still and wider shall thy bounds be set". The website <https://www.nottingham.ac.uk/about/campuses/campus-es.aspx> lists five campuses: University Park, Jubilee, Sutton Bonington, King's Meadow and Malaysia. While it might be a pleasant thought to get away to Malaysia and escape from the seemingly endless cloud and rain we have been having at the time I write this, in fact we shall be heading to the Jubilee campus for our meeting.

If our appetite is whetted by the Spring Meeting, we can further enjoy two specialist meetings in the UK coming up in the next few months. From 25-27 April the second workshop on Dynamic Structural Science will take place at Coseners House, Abingdon. Then, on 15 June, our Industrial Group will hold its XRF meeting at the University of Leicester. Two meetings will appeal to crystallographers with more wanderlust. This year's American Crystallographic Association meeting will be in Denver, CO, from 22-26 July with deadlines of 31 March for abstract submission and 31 May for early registration. About a month later, 28 August – 1 September, the European Crystallographic Association will hold its annual meeting, ECM-30, in Basel, Switzerland. The deadlines here are 6 April for abstracts and 20 April for early registration. We can be proud of our BCA members who will have important roles at these meetings. At the ACA meeting **Elsbeth Garman** will receive the Fankuchen Award "to recognize contributions to crystallographic research by one who is known to be an effective teacher of crystallography" and will deliver the associated lecture (on Tuesday the 26th at 8 AM, so be sure to set your alarm clocks!). With affection and gratitude we know what Elspeth has done for the BCA, but most of us will learn more about her career at the website

<http://www.amercrystalassn.org/2016-award-winners>.

On the preliminary list of keynote speakers at ECM-30 two British crystallographers appear: **Bob Cernik** and **Simon Parsons**. It is up to BCA members to burnish the UK's reputation further by submitting brilliant abstracts!

Powder diffractionists have another opportunity to attend an international meeting in a sunny location. The 15th European Powder Diffraction Conference (EPDIC15) will take place in Bari, in southern Italy near the "heel" of the Italian "boot". The dates are 12-15 June. If you prefer a venue in the USA, you can attend the Denver X-ray Conference – except that this year it will take place in the Chicago area (Rosemont, IL) from 1-5 August. Perhaps they figured that the good people of Denver would be exhausted after an influx of rootin'-tootin'

crystallographers for the ACA meeting, and the next lot ought to go somewhere else!

Back in November, I enjoyed watching the series on BBC4 with the title "Colour: The Spectrum of Science." The third episode extended beyond the visible portion of the spectrum. Dr. **Helen Czerski**, the presenter, went up in a plane with NASA's huge infrared telescope. Attention then shifted to the opposite end of the spectrum, culminating in a lively interview with our own **Anna Warren** and some good background about Diamond.

Last year we joyfully commemorated the 100th anniversary of the awarding of the Nobel Prize in Physics 1915 to **William Henry Bragg** and **William Lawrence Bragg**. Who were the recipients in 1916? It may come as no great surprise that no Nobel Peace Prize was awarded in that dreadful year of conflict. However, no prizes were given that year in Physics, Chemistry, and Physiology or Medicine either. Only the Literature prize was awarded, to the safely home-grown Swedish author Carl Gustaf Verner von Heidenstam. Don't worry: if you wait until next year, X-rays will reappear.

Two pictures of structures on our cover have connections to this year, 2016. Designated the International Year of Pulses by the United Nations, it has connections with the crystal structure of concanavalin A which you can find out about elsewhere in this issue. This year marks the 80th anniversary of the publication by **J. Monteath Robertson** of the crystal structure of phthalocyanine in J. Chem. Soc. 1936, 1195-1209. Aside from the sheer size of the molecule, both the instrumentation for data collection and the methodology for structure solution applied in this paper seem remarkably modern. In his Personal Reminiscences for the IUCr Robertson mentioned that he used the 5 kW rotating anode generator at the Royal Institution (yes, they existed that early!). He recorded the reflected X-rays on films and measured the great majority of intensities with an integrating photometer, not tediously by visual comparison. To solve the structure he noted the isomorphism between nickel phthalocyanine and the free heterocycle and compared the structure factor magnitudes in the presence or absence of nickel. Knowing the location of the nickel atoms, he could work out the phases of the contributions from the heterocycle. Thereby he evolved the heavy atom method and the use of isomorphous substitution.

I conclude by mentioning our cover picture of a record-breaker. In partnership with the International Union of Crystallography, to commemorate the Braggs' Nobel Prize, the Austrian crystallographer and science communicator Dr. **Robert Krickl** assembled a 3 metres tall 3-D model of the crystal structure of sodium chloride. Made of 10 km of sticks and about 40000 little balls, this is the largest model of a crystal's atomic structure ever to be constructed true to scale in 3D. It has been registered with the Guinness Book of Records. The model was proudly displayed in Vienna's city hall last November, where it attracted a lot of interest from the general public, and young people in particular. It appears on a recent issue of Austrian commemorative postage stamps.

Carl Schwalbe

BCA Corporate Membership

The BCA values its close ties with commercial companies involved with crystallography. To enhance these contacts, the BCA offers Corporate Membership. Corporate Membership is available on an annual basis and includes the following benefits:



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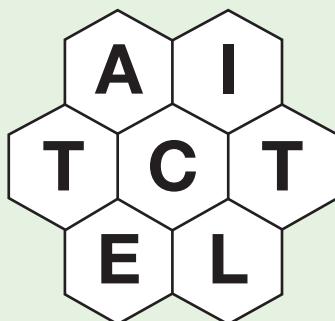
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Puzzle Corner



ALWAYS using the central letter, make words of three or more letters from the letters in the hexagons. Any letter can only be used once. Capitalised words, plurals and conjugated verbs are excluded. Two seven-letter words are possible, one of which is a crystallographic concept. Two shorter words are names for crystalline substances.



Answer to December Puzzle Corner

This puzzle asked you to refer to a well-known compendium, which in this case is the numbered list of space groups. With each number replaced by the first letter of the corresponding Hermann-Mauguin symbol,

H 40 14 4 Y 15 H 155 23 81 196 M 41 82

HAPPY CHRISTMAS. This is not quite right, but trying Schoenflies symbols for the 3 discordant letters gives
HAPPY CHRISTMAS.

BCA Spring Meeting

University of Nottingham, 4-7 April 2016



The University of
Nottingham

From the BCA 2016 Programme Committee

WE look forward to seeing you at the 2016 BCA Spring Meeting, which will be held at the Jubilee Campus, University of Nottingham.

The **Named Lecturers** for 2016 are:

Lonsdale Lecture (Tuesday pm)

Prof. Arwen Pearson (Hamburg)

Visualising molecules in motion: crystallography as a tool to probe structure and dynamics

BCA Prize Lecture (Wednesday pm)

Christer Aakeröy (Kansas State University)

From molecular sociology to functional materials

The **Plenary speakers** are:

BSG: Susan Lea (University of Oxford)

CCG: Mike Zaworotko (University of Limerick)

IG: Rolf Hilfiker (Solvias AG)

PCG: Bill David (Oxford and ISIS)

The majority of speakers for all sessions are now in place. For further, up-to-date details please visit the conference website:
<http://bca2016.crystallography.org.uk>

The Young Crystallographers' Group Satellite Meeting Programme



Monday 4 April, 2016

12:55	Welcome
13:00 – 13:30	Plenary: Prof. Sally Price (UCL) Are polymorphs predictable?
15:30 – 16:00	Plenary: Dr. Andrew Dore (Heptares Therapeutics) StaRs and Structures: An A, B, C of GPCR structural biology and SBDD
17:45 – 18:15	Annual General Meeting
18:30 – 19:30	Session
19.30 – 21:00	Poster Session and Drinks/Buffet

Tuesday 5 April, 2016

09:00 – 10:00	Parkin Prize Lecture: Jonathan Brooks-Bartlett (University of Oxford)
10:10 – 11:30	Forgotten Methods in Crystallography Speaker 1: Mike Glazer (University of Oxford) <i>Plotting three-dimensional information in two dimensions.</i>
	Speaker 2: Paul Raithby (University of Bath) <i>From Films, to Single Point Detectors to Area Detectors – Fundamentals of Diffraction Geometry</i>
	Speaker 3: Bob Eady (University of Liverpool) <i>Protein purification before the His-tag era</i>



Main Meeting Programme

Tuesday 5 April, 2016

12:00 – 12:50

Lonsdale Lecture

Prof. Arwen Pearson (Hamburg)

Visualising molecules in motion: crystallography as a tool to probe structure and dynamics

13:30 – 14:20

CCG Plenary

Chair: Pete Wood (CCDC)

Prof. Mike Zaworotko (Limerick)

Crystal Engineering: Form to Function

14:30 – 16:00

From Amorphous to Crystal [CCG + IG]

Chair: Katharina Focke (Durham University) and

Ghazala Sadiq (CCDC/Pfizer)

This session will cover research into the transitions from amorphous, e.g. solution, glass or gas state, into the crystalline state, the connections between the extremes, and the transition states between them. Special interest is taken in the correlation of these topics with the final crystal structures. This session aims at bridging the fields of pharmaceutical solid-state, organic and inorganic chemistry as well as process engineering, the problems that are encountered in these fields and the solutions that crystallographic methods can offer.

14:30 – 15:00

Keynote: Ivan Marziano (Pfizer)

The Pursuit of the Structure-Function Relationship in Pharmaceutical Crystallization

15:00 – 15:20

J. G. P. Wicker (University of Oxford)

When will it crystallise?

15:20 – 15:40

C. E. Hughes (Cardiff University)

What Can In-Situ NMR Tell Us About Amorphous Intermediates in Crystallization Processes?

15:40 – 16:00

C. D. Jones (Durham University)

Lamellar urea tape networks as building blocks for crystals and gels

14:30 – 16:00

Advanced Functional Materials [PCG]

Chair: Matthias Gutmann (Rutherford Appleton Laboratory)

The development of advanced functional materials is critical to underpinning the development of modern technologies. This session covers such materials with current or potential use in cutting-edge applications. This may include magnetic and electronic materials, such as multiferroics, energy related compounds, for use in solar cells or batteries and modern alloys.

14:30 – 15:00

Keynote: Paolo Radaelli (University of Oxford)

Spins and orbitals in multiferroics: from crystals to devices

15:00 – 15:20

E. Bousquet (University of Liège)

Unveiling the room temperature magnetoelectricity of troilite FeS

15:20 – 15:40

J. W. Bos (Heriot-Watt University)

Variable temperature crystallographic studies of thermoelectric materials with low thermal conductivities

15:40 – 16:00

S. A. Maugeri (Queen Mary University of London)

X-ray and neutron studies of multi walled carbon nanotubes continuously filled with iron

14:30 – 16:00

Antimicrobial Resistance [BSG]

Chair: Ben Luisi (University of Cambridge)

Structural biology is playing a key role in the pursuit of novel strategies to tackle Antimicrobial Drug Resistance (AMR). This session highlights exciting new avenues for novel AMR targets.

Keynote: Prof. Changjiang Dong (UEA)

Transport lipopolysaccharide from the inner membrane to the outer membrane surface

15:00 – 15:30

Dijun Du (University of Cambridge)

Cryo-EM structure of AcrAB-ToIC multidrug efflux pump at near atomic resolution

15:30 – 16:00

K. Beis (Imperial College London)

Structural basis for antibacterial peptide transport across bacterial membranes

16:30 – 18:00

Interactions and Materials [CCG + IG]

Chairs: Graham Tizzard (University of Southampton) and

Cheryl Doherty (Pfizer)

This session will aim to encompass the flourishing and diverse fields of crystal engineering, the design of structures from first principles by directed assembly, as well as the related areas of polymorphism and co-crystal research. This is a joint session between the CCG and IG that will include a broad range of topics of interest to both these communities.

16:30 – 17:00

Keynote: Robert Docherty (Pfizer)

Towards Computational Product and Process Design

17:00 – 17:20

L. R. Agnew (University of Bath)

Towards multi-component templated continuous crystallisation of paracetamol form II

17:20 – 17:40

E. Pidcock (CCDC)

Identifying Relationships between Intermolecular Interactions and Crystal Packing and Symmetry

continued >

17:40 – 18:00

H. H-M Yeung (National Institute of Materials Science)
In-situ Observation of Successive Crystallizations and Metastable Intermediates in the Formation of Metal-Organic Frameworks

16:30 – 18:00

Modelling Crystals and Crystallographic Data [PCG]

Chair: Anthony Phillips

Recent developments in data acquisition, computing power, and our understanding of the fundamental forces at play within crystals have transformed the concept of crystallographic refinement. Among the many “unusual” techniques that are becoming increasingly commonplace are, first, refinement of non-standard parameters: mode amplitudes instead of atomic positions, or thermodynamic properties instead of lattice parameters. Second, refinement against non-standard data is also common: more scattering information than just Bragg intensities, or information from complementary experiments such as NMR or EXAFS, can be incorporated into a crystallographic model. Finally, both empirical and ab initio modelling are increasingly necessary to make sense of complex crystallographic information. This session will focus on using modelling techniques such as these to predict, interpret, and generally get the most out of crystallographic data

16:30 – 17:00

Keynote: Carole Morrison (University of Edinburgh)
Frustrated MOFs: how modelling can help when crystallography can't

17:00 – 17:20

M. Gertsel (Diamond Light Source Ltd)
Coping with volume: Automated data processing on the chemical crystallography beamline I19-1 at Diamond Light Source

17:20 – 17:40

M. J. Cliffe (University of Cambridge)
Correlated defects in hafnium and zirconium MOFs

17:40 – 18:00

P. J. Saines (University of Kent)
Probing the Local Magnetic Structure of a Magnetocaloric Framework, Tb(formate)3

16:30 – 18:00

Developing New Therapeutics [BSG]

Chair: Vilmos Fulop (University of Warwick)

Continuing our theme of AMR, the aim of this session is to showcase the role of structural biology and biophysical methods in developing new protein-based antimicrobial therapeutics.

16:30 – 17:00

Keynote: Colin Kleanthous (University of Oxford)
Import mechanisms of protein antibiotics

17:00 – 17:20

D. Walker (University of Glasgow)
Precision targeting by species-specific antibiotics

17:20 – 17:40

J. Kopec (University of Oxford)
Structural Insights into the MMACHC-MMADHC Protein Complex Involved in Vitamin B12 Trafficking

17:40 – 18:00

C. Bisson (University of Sheffield)
The molecular basis of chiral promiscuity in triazole-phosphonate herbicides that target histidine biosynthesis

18:10 – 19:00

IG Plenary

Chair: Cheryl Doherty (Pfizer)

Dr. Rolf Hilfiker (Solvias AG)

Using Co-Crystals to Optimise Solid Properties

19:00

Buffet dinner, exhibition and posters.

Wednesday 6 April, 2016

09:00 – 09:50

BSG Plenary

Chair: Simon Newstead (University of Oxford)

Prof. Susan Lea (University of Oxford)

The use of hybrid structural methods to study the protein complexes required for export of proteins from bacteria

09:50 – 10:15

Coffee break

10:15 – 11:45

Future of Structural Science [BSG]

Chair: Alex Cameron (University of Warwick)

10:15 – 10:45

Keynote: Xiaodong Zhang (Imperial College)

Structures and Mechanisms of Bacterial RNA Polymerase Inhibition and Activation by sigma54 and its AAA activators

10:45 – 11:05

B. Luisi (University of Cambridge)

Title TBC

11:05 – 11:25

J. Helliwell (University of Manchester)

Access to raw diffraction data; current practice in article linking to raw diffraction data

11:25 – 11:45

M. Bowler (European Molecular Biology Laboratory)

Structural basis for the subversion of MAP kinase signalling by an intrinsically disordered parasite secreted agonist

10:15 – 11:45

NMR Crystallography [CCG]

Chairs: Gareth Lloyd (Heriot-Watt) and Paul Hodgkinson (Durham)

Nuclear Magnetic Resonance (NMR) Crystallography uses the exquisite sensitivity of NMR frequencies to local environment in order to elucidate crystallographic information. DFT-based methods now allow NMR measurements to be directly correlated with molecular packing, and a range of NMR experiments can be used to probe questions of disorder, dynamics, structure and crystallography.

10:15 – 10:45

Keynote: **Yaroslav Khimyak** (University of East Anglia)
Understanding structure of molecular organic solids: combining crystallography with insights from NMR

10:45 – 11:05

K. Johnston (Durham University)
Studying Transition-Metal Organometallic Complexes using Diffraction, ³⁵Cl Solid-State NMR and First-Principles DFT Calculations

11:05 – 11:25

A. C. Poepller (University of Warwick)
“Good Cop and Bad Cop” – NMR Crystallographic and Powder X-ray Analysis of Lithium and Magnesium Orotate Hydrates

11:25 – 11:45

A. Morris (University of Cambridge)
High Throughput Crystal Structure Prediction: Using NMR and DFT to design Phosphorus Electrodes for Li and Na-Ion Batteries.

10:15 – 11:45

Structure and Function (Ad Hoc Session)
Chair: Richard Cooper (University of Oxford)

10:15 – 10:45

Keynote: **A. J. Blake** (University of Nottingham)
High pressure coordination chemistry and the search for new phenomena

10:45 – 11:05

A. E. Phillips (Queen Mary, University of London)
Disorder in metal-organic frameworks from total neutron scattering

11:05 – 11:25

E. M. Reynolds (University of Oxford)
Structure-property relationships of Tc-containing perovskite oxides

11:25 – 11:45

P. A. Corner
Applying an Optimised Co-crystal Screen Utilising Ultrasoundication to Active Pharmaceutical Ingredients

12.15 – 12.45: CCG Annual General Meeting

12.15 – 12.45:

12.45 – 13.15: PCG Annual General Meeting

12.45 – 13.15:

13:30 – 15:00

Early Career Prize Session

CCDC Chemical Crystallography Prize for Younger Scientists 2016

Dr. Mark Warren (Diamond Light Source)

15:00 – 15:30

Coffee break

15:30 – 17:00

Future of Structural Science [PCG]

Chair: Mike Glazer (University of Oxford)

In the last few years important advances have been made in techniques to investigate the structures of crystals and molecules. In particular the advent of the free electron laser has shown that it is possible to gain structural information on macromolecules without the need to grow large single crystals. Another area of advance is in the field of electron microscopy, where the development of new aberration-free lenses enables individual atoms to be imaged; the use of freezing methods as in CryoEM enable at least protein molecules to be imaged even when not in crystalline form. Alongside the rapid advances in other experimental and computational techniques this raises key questions about the nature of the future of structural science including whether in the future crystals will be needed at all. It is time that crystallographers think about this and consider the impact of these new techniques on their subject.

15:30 – 16:00

Keynote: **John Spence** (Arizona State University)
Opportunities for structural biology using X-ray lasers

16:00 – 16:20

D. A. Keen (Rutherford Appleton Laboratory)
The future of structural science – does neutron diffraction have a role?

16:20 – 16:40

P. Wood (CCDC)
The future of structural databases

16:40 – 17:00

SPEAKER 3

15:30 – 17:00

Complementary Techniques [CCG]

Chairs: Helena Shepherd (University of Kent) and Andrew Stewart (Limerick)

There are many techniques that can give complementary information to traditional crystallographic approaches. This session will explore the use of techniques including computational studies, electron diffraction and microscopy, spectroscopy and scattering to allow a more complete understanding of the molecules and materials we study.

15:30 – 16:00

Keynote: **Graeme Day** (University of Southampton)
Energetic aspects of molecular crystals: from polymorphism to prediction

continued >

16:00 – 16:20

A. M. Reilly (CCDC)

6th Blind Test of Organic Crystal-Structure Prediction Methods: Overview & Predicting Structures with CSD Analogues

16:20 – 16:40

S. P. Gurung (University of Reading)

X-ray Crystallographic and Photophysical Studies of DNA i-motifs

16:40 – 17:00

C. L. Hobday (University of Edinburgh)

Tuning the Gate Opening Pressure of Zeolitic Imidazolate Frameworks

15:30 – 17:00

Application of Crystallography to Crystal Growth [BACG + IG]

Chair: Neil Feeder (CCDC)

15:30 – 16:00

Keynote: **Roger Davey** (University of Manchester)

The application of crystallography to problems of crystal growth

16:00 – 16:20

C. Seaton (University of Bradford)

Controlling Crystal Forms of Chiral Materials: The Role of Heteromolecular Interactions

16:20 – 16:40

W. Z. Zhou (University of St Andrews)

Non-classical Crystal Growth of Some Solid State Materials

16:40 – 17:00

SPEAKER 3

17:10 – 18:00

BCA Prize Lecture

Christer Aakeröy (Kansas State University)

From molecular sociology to functional materials

18:00 – 19:00

The Annual General Meeting of the British Crystallographic Association

19:30 for 20:00

BCA Conference dinner

Thursday 7 April, 2016

09:00 – 09:50

PCG Plenary

Chair: Phil Lightfoot (University of St Andrews)

Prof. Bill David (ISIS Facility, University of Oxford)

120 Years of Powder Diffraction

09:50 – 10:15

Short break

10:15 – 11:45

Phase Transitions [PCG]

Chair: Christoph Salzmann (University College London)

Phase transitions are at the very heart of solid-state chemistry, crystal engineering and mineralogy. The aim of this session is to cover as many aspects of this important phenomenon as possible including phase transitions between crystalline as well as amorphous materials. Particular emphasis will be put on the real-time and in-situ detection of phase transitions as well as the description and parameterisation of symmetry changes.

10:15 – 10:45

Keynote: **John Evans** (University of Durham)

Phase Transitions and Symmetry Mode Analysis of Functional Materials

10:45 – 11:05

C. J. McMonagle (University of Edinburgh)

High-Pressure Guest Included Phase Transitions, Amorphisation and Negative Linear Compressibility on a Porous Copper-Based Metal Organic Framework

11:05 – 11:25

A. R. Palliparuth (National University of Ireland, Galway)

Understanding polymorphism and phase transformations in Diflunisal and the role of hydrogen bonding in tailoring crystal habits of its co-crystals

11:25 – 11:45

J. K. Cockcroft (University College London)

A variable temperature study of long chain alkyl trimethyl ammonium bromides combining SXD and PXRD methods: Crystallographic pitfalls for the unwary and structural surprises!

10:15 – 11:45

Tips, Tricks and Trials [CCG]

Chairs: Mike Probert (Newcastle) and Iain Oswald (Strathclyde)

This session will aim to span the crystallisation journeys of various samples through to the measurement of their diffraction patterns, aiming to explain various Tips Tricks and Trials that the speakers have employed under different circumstances.

10:15 – 10:45

Keynote: **David Allan** (Diamond Light Source)

Growing Crystals at High Pressure

10:45 – 11:05

P. Shaw-Stewart (Douglas Instruments)

Microseed matrix-screening (rMMS): introduction, theory, practice and a new technique for membrane protein crystallization in LCP

11:05 – 11:25

H. Puschmann (Durham University)

The Pesky CIF -- and how to tame it

11:25 – 11:45

N. Johnson (Newcastle University)

The Integration Game: Data Processing for Small Molecule Crystallography

10:15 – 11:45

Structural insights into Cell Processes [BSG]

Chair: Neil McDonald (The Francis Crick Institute)

Proteins operate in dynamic networks of interactions and pathways. The aim of this session is to highlight the advances made in understanding dynamic cellular networks, such as phosphorylation and neuronal signalling, using state of the art crystallographic techniques.

10:15 – 10:45

Keynote: Richard Bayliss (University of Leeds)

Protein Kinases and their On and Off Relationships

10:45 – 11:05

Radu Aricescu (University of Oxford)

Crystal structure of a human GABAA receptor

11:05 – 11:25

E. Seiradake (University of Oxford)

Super-complexes of adhesion GPCRs and neural guidance receptors

11:25 – 11:45

D. Briggs (Imperial College London)

12:00 – 13:30

Local Structure-Property Relationships [PCG]

Chair: Helen Playford (Rutherford Appleton Laboratory)

The local structure of materials often plays a critical role in determining their properties yet cannot be perceived easily by conventional crystallographic analysis; this is particularly pertinent in amorphous and nanocrystalline systems which lack the requisite long-range order. This session will focus on materials where such understanding of the local structure is vital, discussing results from techniques sensitive to these length-scales, such as Pair Distribution Function (PDF) data, Extended X-ray Absorption Fine Structure (EXAFS) spectroscopy, diffuse electron scattering and computational modelling. Where possible, it will highlight the complementary nature of these techniques and the way in which they can be combined to address difficult problems.

12:00 – 12:30

Keynote: Ian Reaney (University of Sheffield)

Local structure-property relations in perovskite structured ceramics

12:30 – 12:50

J. J. Shephard (University College London)

Validation of diffraction-derived structural models of liquids using dielectric spectroscopy and vapour pressure measurements – Are we even in the ball park when it comes to local structure in liquid chloroform and the mixing characteristics of chloroform-acetone and benzene-methanol azeotropes?

12:50 – 13:10

P. M. Thygesen (University of Oxford)

Orbital dimer model for spin glass state in Y₂Mo₂O₇

13:10 – 13:30

L. R. Owen (University of Cambridge)

Short range order in metal alloys

12:00 – 13:30

Would you publish this? [CCG + YCG]

Chairs: Pascal Parois (Oxford) and Jorge Sotelo (Edinburgh)

Following last year's success, this interactive session of unusual format is aimed for discussing problematic crystal structures that can be hard to interpret and publish. After an opening talk on the challenge of publishing difficult structures, anyone present can briefly describe one or more structural results that raise the session title question for the audience to discuss, with the aim of constructive rather than negative criticism. Problems might include charge imbalance or other chemical issues, poor resolution or data completeness, complicated disorder, highly restrained models, unexplained residual electron density and other artefacts, etc. A formal abstract is not required, but please contact the session organisers in advance of the meeting (as soon as possible!) if you wish to contribute; we will request 1–3 slides for concatenation into a single session presentation. Contributions from Young Crystallographers are particularly encouraged.

12:00 – 12:30

Keynote: Iain Oswald (University of Strathclyde)

Pharmaceuticals... I thought they were meant to make you feel better!?!?

12:00 – 13:30

Molecular Machines [BSG]

Chair: Susan Lea (University of Oxford)

In the past couple of years substantial progress has been made in our understanding of how protein dynamics operate at the molecular level. The aim of this session is to highlight recent advances in our understanding of these systems and showcase several important advances from UK laboratories in this field.

12:00 – 12:30

Keynote: Neil McDonald (The Francis Crick Institute)

Structural insights into growth factor signalling and cell polarity

12:30 – 12:50

H. Schmidt (MRC Laboratory of Molecular Biology)

The pre-and post-power stroke crystal structures of the dynein motor domain

12:50 – 13:10

J. Emsley (University of Nottingham)

Title TBC

13:10 – 13:30

K. Goodman (Columbia University)

Molecular logic of clustered protocadherin-mediated neuronal self-recognition

continued >

Workshop Programme – “Crystallisation – Tips and Tricks”

Chair: Horst Puschmann (Durham University)

Tuesday 5 April, 16:30 – 18:00

Katherina Edkins (Durham)

Theory and introduction to crystallization

Mark Elsegood (Loughborough)

These crystals will make your crystallographer happy

Wednesday 6 April, 10:15 – 12:15

Jona Foster (Sheffield)

Crystal growth in gels

Dmitry Yufit (Durham)

In-situ temperature-induced crystallisation

Mike Probert (Newcastle)

In-situ pressure-induced crystallisation

The BCA 2016 Programme and Organising Committee is:-

Phil Lightfoot (Chair)

Alex Cameron (BSG)

Simon Newstead (BSG)

Mark Roe (BSG)

Pascal Parois (CCG)

Lynne Thomas (CCG)

Qendresa Osman (IG)

Ghazala Sadiq (IG)

Nicholas Funnell (PCG)

Paul Saines (PCG)

Horst Puschmann (Workshops)

Scott McKellar (YCG)

Natalie Johnson (YCG)

Lee Brammer (BCA President)

Richard Cooper (BCA Vice President)

Claire Wilson (BCA Secretary)

Pamela Williams (BCA Treasurer)

Phil Lightfoot

Chair of BCA 2016

pl@st-and.ac.uk

&

Richard Cooper

BCA Vice President

richard.cooper@chem.ox.ac.uk



2016 AGM

THE 2016 Annual General Meeting of the British Crystallographic Association will be at the University of Nottingham at 18:00 on Wednesday 6th April, 2016.

Elections

Elections for several positions on Council will be held at the AGM: the Vice-President (**Richard Cooper**) and the secretary (**Claire Wilson**) each complete a 3 year term and one ordinary member (**Andrea Thorn**) completes a 3-year term.

Nominations for any of these vacancies may be made by any two members and should be accompanied by the written consent of the candidate to serve if elected.

Nominations must be received by the Secretary (secretary@crystallography.org.uk) not less than 4 days before the AGM (i.e. by April 1st 2016).

Draft Agenda

- 1) Approval of Agenda
- 2) Apologies for Absence
- 3) Minutes of last AGM
- 4) President's Report
- 5) Secretary's Report
- 6) Hg3 Report
- 7) Report of the Treasurer to include Presentation of the Accounts for 2015 and the Examining Accountant's Report
- 8) Acceptance of the Accounts
- 9) Appointment of Examining Accountant for 2016
- 10) Elections to Council
- 11) Honorary Members
- 12) Membership, annual subscriptions and subventions
- 13) Any other business



Draft minutes of the BCA Annual General Meeting 2015

PX001, University of York, 18:00 1st April 2015.

1. Approval of Agenda

Proposed by Sandy Blake and seconded by Elspeth Garman.

2. Apologies for Absence

None received.

3. Minutes of the last AGM

Claire Murray proposed and Andrea Thorn seconded the approval of the minutes.

4. President's report

The President noted the death of Frank Allen who died in November 2014 and was known to many of the BCA membership, was an Honorary member of the BCA and is sadly missed.

The current spring meeting is an excellent celebration of crystallography and he thanked the programme chair John Helliwell, Richard Cooper and Hg3. The BCA Spring meeting 2016 will be held at the University of Nottingham, Jubilee Campus from 4th-7th April and the Programme Chair is Phil Lightfoot.

The President highlighted the BCA website and thanked those responsible. He also drew attention to some of the highlights of the public engagement events and crystallography in the news during the last year, including the Big Bang Fair, Gravity Fields, Elspeth Garman on the radio, good links with STFC and Diamond and the learn.crystallography.org.uk website. The Illuminating atoms exhibition was shown in the Royal Albert Hall and the President thanked Max Alexander, the photographer, and Clare Murray, for organising this. He also noted that the President elect of the Royal Society is Sir Venki Ramakrishnan. Thanks were given to Sam Callear as Education and Outreach coordinator and also to all volunteers involved. He also highlighted the BCA twitter account. Thank you to BCA officers and Council and webmasters, Crystallography News editor, Nicola Peel from Hg3. All members of the BCA were thanked for their continued support of the Association and he concluded by commenting that he had enjoyed his presidency.

5. Secretary's report

There was nothing to report and no questions.

6. Hg3 report

Nicola Peel gave her report. There are 683 members this year compared to 696 at this time last year and a breakdown of figures for each of the membership

categories was given in presentation. There are 11 corporate members including a new member, Bio-Rad, and we welcomed them on board. Crystallography News is about breakeven and Nicola commented on the balance needed between postage costs and pdf version and whether they were as attractive to advertisers as advertising is very valuable. There are 6 advertisers.

Spring meeting numbers are up this year (200 full registration, 15 day registrations, 250 attendees in total) and the exhibition space has been buzzing and exhibitors are happy. There are 20 exhibition stands this year with a revenue of £12,740 compared to 15 last year (revenue £11,460); the revenue increase is not proportionate to number of exhibitors which reflects a number of small stands.

7. Treasurer's report

Printed copies of a summary of the accounts were circulated in the meeting and the Treasurer indicated that the full accounts are available via email or online through the charity commission website. She also clarified that the accounts are given for a calendar year, in this case Jan 1st to Dec 31st 2014. Our membership subscriptions have increased to £19,860 compared to £14,662 in 2013. For other comparisons it should be noted that 2013 was a good year for the BCA finances as there was a surplus from the ECM in Warwick and it was unusual as there was no Spring meeting. Crystallography News totals vary from year to year due to differences in when items billed for and paid fall.

Our running costs for the organisation are ~£13,000 a year includes membership administration, insurance, and accountancy costs. Therefore there is not a huge difference between the membership income and governance costs. A question was asked regarding why the governance costs had dropped so much compared to 2012. This reflects the change from Northern Networking (NN) to Hg3; we were spending a lot more administration fees and now have far more transparency in costs from Hg3. Elspeth Garman commented that NN were paid a flat fee and had no intrinsic interest in maintaining membership numbers whereas Hg3 have a fee linked to the number of members and so have much more interest in chasing this up.

For Spring meeting 2014 the number of delegates was lower and this is the main reason for the loss. Outgoings include our subs to IUCr (CHF 15000) and ECA membership (560 euros). The Royal Society currently pay 49% of the IUCr subscription. Crystallography News revenue should be higher this year (2015). We continue to give out bursaries to attend meetings. Keith Wilson asked how many delegates we aimed to have at the Spring meeting. In the past the Spring meeting has been a source of income but not last year when there was a loss. The

Treasurer reported that we had aimed for a breakeven of 250 delegates and the President commented that we had deliberately set a relatively high number to aim for. In future the BCA aims to make at least a small surplus on the meeting. The outcome of this meeting will not be known for another week or so. Sandy Blake asked whether it was known why the numbers were reduced for the Loughborough meeting as there was a good programme and commented that there was some difficulty with the dates being in term time for some people. One possibility was that the ECM took place in the UK the August 2013 just before that Spring meeting.

The Treasurer encouraged members to tell Council or their Group committees if they had suggestions of venues or other ways that the meetings can be improved. Matt Tucker suggested that we canvass the members who do not attend the Spring meeting, for example via an email questionnaire and Dave Keen encouraged members present at the meeting to ask colleagues who hadn't attended about their reasons and email us.

Last year there was a total dip in our funds of around £13,000 and we want to continue to award bursaries and sponsor events including outreach activities but are mindful that we are currently running at a loss and longer term that isn't sustainable.

Thanks were given to Hg3, Council members, Group treasurers, Charles Stanley Bank and The Young Company accountants.

8. Acceptance of the accounts

This was proposed by Pierre Rizkallah and seconded by Dave Allan and approved.

9. Approval of the Examining Accountants for 2015

The appointment of the Young Company, with a fee of £4,800, as for last year, was proposed by Mike Glazer and seconded by Ed Bilbé and approved.

10. Membership, Annual Subscriptions and Subventions

The President gave a short presentation to explain some of the options to adjust our income and expenditure. As reported above the BCA is currently running at a loss and although it is not urgent to address this, as the organisation has reserves, it is not sustainable in the long term.

Membership fees were last increased in 2012 and any decision today would be for fees for the following year (2016).

The BCA council brought to the AGM a proposal to reduce the IUCr category of adherence from the current category V to category IV. A document was circulated to all the BCA members, with the agenda and minutes from last year's AGM, outlining the IUCr subscriptions and the levels of adherence. The President talked through this explaining that the UK is currently a category V adherent with 5 votes at the general assembly and had confirmed that otherwise all members have equal rights within the IUCr. The subscriptions are linked to the level of adherence but not linearly so that a category IV adherent pays 10 units

(CHF1000 per unit) whereas a category V adherent pays 15 units. As the charge is in Swiss francs then it is also subject to exchange rate changes which changed by ~10% this year. The President corrected the figure given previously as a 5-fold increase in the circulated document and clarified that this had been due a change in accounting for this which now gave the total cost including the Royal Society contribution and is in fact ~1.6 fold increase. The cost to the BCA this year is ~£5.5k and the cost per member £9 (30% of full membership and 60% of concessions). There are 91 votes from 50 adherents.

Mike Glazer, Vice President of the IUCr, provided some background to the meeting and explained that the issue had been raised at the IUCr finance committee and there had been proposals to either give the cost in another currency or to reduce the unit cost for everyone. It had been close to being agreed to reduce the cost but wasn't passed. He reported that he intended to take this back to the next meeting in Croatia in August 2015.

There was a discussion involving many of the membership on the matter of how a change of the level of adherence to IUCr might affect the BCA's standing internationally and its influence within the IUCr, and how this would be balanced by the cost saving. It was commented that the fact that this was being raised may give more power to Mike Glazer when returning to the IUCr finance committee. It was also commented that there isn't an urgent need to cut costs as this point as there are reserves. The possibility to increase income through membership fees and address whether there are alternative routes to increasing our income through additional corporate members etc. was also commented on.

The President commented that there is a need to balance the considerable heritage of the UK and our financial means. It was also clarified that there was no suggestion of leaving the IUCr and no question of the value of the organisation, but rather of what level of adherence is appropriate for the BCA. BCA council has a responsibility to bring this possibility to the membership.

It was noted that the BCA strongly supported Mike Glazer's attempts to address this with the IUCr.

A vote was taken and the motion was not carried. The BCA membership voted to remain a category V adherent to the IUCr.

BCA Council brought to the AGM for approval a proposal of an increase of £5 for full membership subscription to the BCA and a pro-rata increase for other membership categories bringing the fees to £35 for full membership, £17.50 for concessions, £58.50 for 4 year student membership and £175 for a 5 year overseas membership. This was approved.

It was clarified that with this increase in membership fees, and no change to the IUCr adherence level, assuming other things were unchanged that the BCA would still be running at a small loss.

An informal vote was taken as to whether the members were in favour of a further increase next year. A show of hands indicated a majority in favour.

11. Elections to BCA Council

The following positions on council were due for election:

President – Lee Brammer nominated by Mike Glazer and seconded by Richard Cooper.

Education and Outreach Coordinator – Simon Coles nominated by Mike Hursthause and seconded by Claire Wilson.

Ordinary Council Member – Mark Senn nominated by Simon Parsons and seconded by Richard Cooper.

In all cases the nominations were unopposed and the nominees were duly elected.

12. Honorary Members

The President clarified that Honorary members of the BCA are chosen for their contributions both to crystallography and to the BCA. They may be proposed by any member by sending a recommendation to the President who, usually after consultation makes the decision on any new Honorary members. An Honorary member retains their membership for life and their number is limited at any one time. Members were encouraged to consider any nominations for new Honorary members for 2016.

13. A.O.B.

Mike Glazer proposed a vote of thanks to Dave Keen for the last 3 years as President for doing a very good job.

The meeting closed at 19:40.

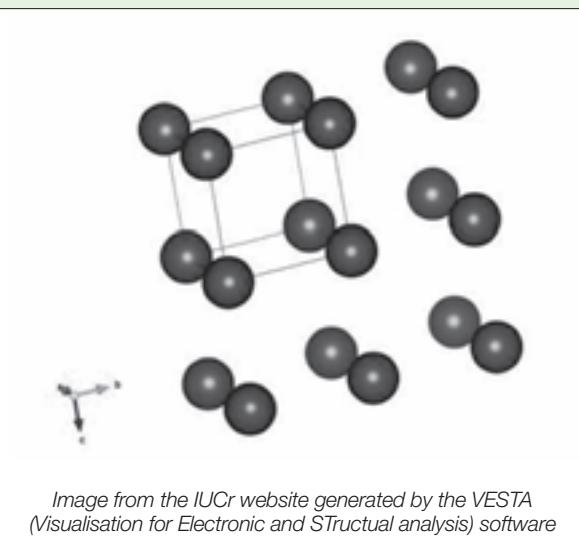


Polonium: Structure of the Day for 5 February

THE www.iucr.org website is always educational. If you look near the top of the right-hand column, it can provide entertaining diversions as well. There you will find the Structure of the Day, one of 365 that were curated for the International Year of Crystallography by our own Helen Maynard-Casely and are still on display now. I call Helen “our own” because she did her PhD and postdoctoral research in Edinburgh, winning the Panalytical PCG Thesis Prize in 2010 and giving the Parkin Lecture in 2011. Now she is at ANSTO, appropriately working on an instrument called WOMBAT. Spare a thought for her, parched in the heat of an Australian summer rather than being well hydrated in Edinburgh!

Because polonium poisoning was in the news again recently, this entry particularly caught my eye. The interest in polonium goes well beyond its use as a poison in the shadowy world of political assassination, and the romance of its discovery by Marie and Pierre Curie, who extracted it from tons of mining waste in a draughty shed in Paris. Polonium is unique among the elements in that it has a simple cubic structure, not a close-packed one. Its atoms sit directly on top of the atoms in the layer below rather than reposing in the dimples between them. Theoreticians have attributed the unexpected stability of this arrangement to the relativistic mass-velocity and Darwin energy terms.

Carl Schwalbe



BCA-BSG / CCG / IG / YCG Group Meetings

BCA/BSG Winter Meeting



THE BSG Winter meeting was held in the MIB at Manchester on Wednesday 16th December with the title "Reactive Macromolecules". There were six speakers and the programme attracted people from all points of the country – from Brighton to Edinburgh and Cardiff to Norwich.

The first talk was given by **Karl Payne** who spoke about the UbiD/UbiX system that they are using to produce hydrocarbons for fuel from biological materials. He showed that normally expressed UbiX contains a FMN cofactor, but when it is co-expressed with UbiD then the cofactor is altered with the addition of DMAP to the FMN and it is this cofactor that allows the UbiX to decarboxylate its substrates. These results were corroborated with very high resolution crystal structures. The second talk was presented by **Roberto Steiner** on the Urate Oxidase system. His talk showed the perils of radiation damage in interpreting biological data – data collected at the synchrotron showed no peroxide formation, in contrast to in-house collection that showed the peroxide clearly (again with high resolution structures). He also showed data following the reaction spectroscopically and showed that the oxidation reaction was not 1st order, so that it must go through a peroxide intermediate.

The first talk after lunch was given by **Tom Clarke** on Multiheme Metal Reductases. He first showed the usual respiration sequence, which is dependent on small molecules and leads to energy production and then showed that bacteria living on minerals must utilise a different pathway as minerals are not diffusible. He showed the first structure of MtrF – a very difficult problem with 87% solvent, solved by using Fe-SAD from 10 haems. Further work in reconstructing the electron transport system in liposomes showed that direct contact from the surface cytochromes to the mineral surface dominates the metal reduction process. **Richard Pickersgill** gave the next talk, entitled Enzyme Traps, and showed us two types of 'trap'. Firstly he gave a detailed description of the cobalamin biosynthetic pathway (with structures for many of the steps) and showed that often the product of a reaction was trapped until the next enzyme in the pathway released it – presumably to avoid side reactions and product loss. He also introduced Bacterial Microcompartments which are protein compartments that trap enzymes – the most famous being the carboxysome which traps RuBisCo and Carbonic Anhydrase. This is probably for kinetic or thermodynamic reasons or, again, to reduce unwanted side reactions.



(L-R) Pierre Rizkallah (Chair #2); Richard Pickersgill; Yvonne Jones; Lydia Tabernero (Chair #3); Karl Payne; Tom Clarke; Mathew Martin; Roberto Steiner.

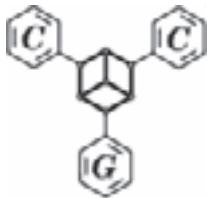
After tea, **Yvonne Jones** gave a talk on how Wnt signalling is controlled, showing how Wnt brings together Frizzled and Wrp5/6 to start the Wnt signalling. She then showed how Wnt binds to the ectodomain of Wrp5/6 via a pincer with its finger and palmitoylated thumb. Then she introduced Norrin which also binds Frizzled (and can activate the Wnt pathway), but only when SOS (a proteoglycan mimic) is used and also Notum which is an inhibitor of Wnt signalling and showed that this was because the Notum removes the palmitoyl from the Wnt disrupting its binding to Wrp5/6. The last talk was given by **Matthew Martin** on Serendipitous Drug Discovery. He showed how many proven kinase inhibitors can also inhibit bromodomains. He showed several structures and pointed out that the kinase inhibitors were using several different binding modes to inhibit the bromodomains.

Mark Roe
University of Sussex



The Poster-Prize (sponsored by IUCr) is presented by **John Helliwell** to **Christopher Earl** of the Birkbeck/UCL Institute of Structural and Molecular Biology (Chris is based at Birkbeck College).

Chemical Crystallography Group Autumn Meeting



THIS year's CCG Autumn Meeting was entitled "Functional Materials" and held at the Strathclyde Institute of Pharmacy and Biomedical Sciences (SIPBS) in Glasgow. This one-day meeting offered a genuinely excellent line-up of speakers covering a fascinating cross-section of science on functional materials. During the day we touched upon crystallisation and gelation, nanoporous materials, pharmaceuticals as well as dynamic reactions and transformations within materials. We are very grateful to Rigaku Oxford Diffraction for their kind sponsorship of this meeting and also to the CCDC to providing additional sponsorship.

After the opening remarks from **Peter Wood** (CCDC), the meeting proper started with **Jon Steed** (University of Durham) who had the intriguing title of "Sliding Down the Supersaturation Gradient: Crystals, Gels, Drugs and Blue Ketchup". He discussed the factors that affect the supramolecular self-assembly of a range of low molecular weight gelators and ways in which the gelation can be switched on and off. This included using ionic additives such as metal salts or chloride anions. Crystal engineering approaches can be used to change the macroscopic physical properties such as the behaviour under applied stress and this included familiar intermolecular interactions such as hydrogen bonding and halogen interactions. Gels are also a useful tool for controlling crystallisation including templating metastable crystalline forms of pharmaceuticals. The on-off nature of the gels makes it possible to recover the crystalline product.

Valeska Ting (University of Bath) moved us from the small-scale production of solid materials to an engineer's approach applied to hydrogen storage materials. There are a number of assumptions which engineers apply to their materials including assuming that there is no thermal expansion between 77K and room temperature. Using X-ray and neutron diffraction, it is possible to follow the gas loading of a range of different metal-organic frameworks (MOFs), to investigate, in detail, the expansion behaviour of the materials and to test out some of the limitations of the current engineering approaches to hydrogen storage materials.

After lunch, **Ross Forgan** (University of Glasgow) kicked off the afternoon's sessions with an excellent overview of his group's research improving the synthesis, crystallinity and mechanical stability of MOFs. Solvothermal synthesis of MOFs typically uses significant quantities of a modulator compound (often a simple carboxylic acid) though the exact function of this modulator is not well understood. Ross showed that careful selection of the modulator can have a dramatic effect on crystallinity. The use of L-proline as a modulator proved particularly effective in the case of one MOF they were working on, so effective in fact that good quality single crystals could be obtained. The availability of good quality single crystals also means that more in-depth structural studies can be performed



Ross Forgan from the University of Glasgow.
Picture courtesy of Valeska Ting (University of Bath).

on a given MOF, such as high pressure analyses and even single crystal to single crystal bromination transformations.

Jonathan Burley (University of Nottingham) next introduced us to the concept of using Raman spectroscopy for solid form screening. Apparently improvements in semiconductor light detector technology in recent years have massively increased the potential of Raman spectroscopy in this area. Jonathan has shown that it is possible to get usable data characterising the solid form of a sample in a hundredth or even a thousandth of a second. It is possible now to distinguish between different polymorphs of a compound as well as to distinguish crystalline samples from amorphous ones using Raman. The technology seems very well set up for application in solid form screening of drugs at very small scale.

After coffee, the final session began with **Kim Jelfs** (Imperial College) explaining how to predict both structure and function in porous molecular materials. The two main focusses of this work are towards ensuring synthesisability of the predicted materials and finding those with genuine, usable porosity. The aim is to be able to move from a 2D sketch of the material through to a reliable 3D structure with calculated properties to ensure less wasted synthesis time. One of the main challenges is to take into account the solvent within the pores – if the solvent molecules are not considered, the 3D structures tend to collapse in the calculations. The approach developed in the Jelfs group is facile and can be applied across a range of systems of interests including metal organic frameworks (MOFs) and covalent organic frameworks (COFs).

continued >



Kim Jelfs from Imperial.
Picture courtesy of Valeska Ting (University of Bath).

The meeting was concluded by **Lee Brammer** (University of Sheffield) who nicely drew the meeting together by running us through chemical reactions and dynamic processes occurring all the way through from molecular crystals to framework materials. This included materials which possess porosity without pores and utilised coordination chemistry and intermolecular interactions such as halogen bonding. The value of using *in situ* and complementary measurements to follow these complex reactions was demonstrated and shown to be necessary to fully understand and develop the processes.

The meeting ended as it had begun as the delegates departed into some of Glasgow's finest liquid sunshine!

Peter A. Wood (CCDC) & Lynne Thomas (University of Bath)

from **Andrew Bond** from the University of Cambridge. Andrew outlined his extensive research in the field of crystal engineering, utilising it for enhanced property control. He went on to discuss the implications of polytypism, using the examples of aspirin, piroxicam and felodipine, demonstrating the ability of nanoindentation techniques for distinguishing between such forms.

Andrew was followed by **Andy Stewart** from the University of Limerick. He presented his extensive work in the field of electron diffraction tomography, a useful technique for structure determination using crystals of insufficient size for X-ray diffraction. Current advances include the structure determination of carbamazepine from a 10nm crystal, demonstrating the advantages of electron diffraction for allowing detection at the very limits of crystallinity.

The day concluded with "Complementary Tools in Pharmaceuticals", chaired by **Les Hughes** (AstraZeneca).

Steve Cosgrove, also from AstraZeneca, reminded us of the importance of understanding the link between structure and properties. He laid out the uses of structural informatics in the context of the pharmaceutical journey, presenting examples from AstraZeneca.

Steven P. Brown from the University of Warwick completed the lecture programme with his talk about NMR crystallography. He demonstrated the advances in solid-state NMR in conjunction with the pharmaceutical industry, outlining the applications of two-dimensional ^1H , $^{1\text{H}}\text{-}^1\text{H}$ double quantum and ^{14}N - ^1H experiments for the identification and characterisation of intermolecular interactions within solid structures. This was outlined with examples of indomethacin as well as in indomethacin-nicotinamide co-crystals.

Overall, it was a very informative and enjoyable day. Thank you to the organisers and the sponsors: AstraZeneca, Bruker and Pfizer.

Alex Cousen, Ruth Lunt and Anneke Klapwijk (University of Bath)

Industrial Group Autumn Meeting



THIS year's Industrial Group Autumn meeting took place on 12th November 2015 and was held at AstraZeneca, Macclesfield. The day consisted of seven talks from various academic and industrial speakers, themed around the issue of "Cracking Challenging Crystals".

The first session, chaired by **Helen Blade** (AstraZeneca), was entitled "Crystallisation Control" and began with a talk from **Nick Blagden** from the University of Lincoln. His work outlined the use of micro channels for anti-solvent crystallisation, highlighting the importance of channel design in the control of liquid-liquid interfaces, a key parameter for particle development. In tandem to this, he also spoke about the challenges of using surfactants in order to further control crystal growth.

Next, **Iain Oswald** from the University of Strathclyde discussed the use of anti-solvent crystallisation in the production of multi-component species of L-amino acids, the solid-solutions of which were shown to have subtle differences in their infra-red spectra. The bulk production of such systems was then developed through the use of continuous anti-solvent crystallisation.

The morning session concluded with **Kenneth Lewtas** from Lewtas Science & Technologies Ltd. Kenneth spoke about his background in a variety of fields, discussing the use of specific crystal modification additives for a range of applications. His work focused on the control or prevention of crystallite formation, arching over several industries including pharmaceuticals, diesel fuels, adhesives and polymers.

After a hearty lunch, the session on "Structure Solution", chaired by **Cheryl Doherty** (Pfizer), was opened by a talk

The Young Crystallographers Group



The Young Crystallographers Group is currently in the process of organising what we are sure will be an interesting satellite meeting on the 4th and 5th April, at the University of Nottingham, directly before the BCA Spring Meeting. There has been a consistently positive response from all corners of the crystallographic community in previous years and we trust that this year will be no different. Both Plenary speakers are confirmed:

Prof Sally Price (UCL) will be opening the meeting, questioning “Are polymorphs predictable?”, while Dr Robin Owen (I24, Diamond Light Source) will be later discussing “New approaches for microfocus crystallography at Diamond and beyond: from smaller beams to serial delivery”. On the second day, the closing session is this year entitled “Forgotten Methods in Crystallography”, where we will see three experienced academics passing on knowledge at risk of being lost to the younger generation of scientists. Prof Paul Raithby (University of Bath) will discuss detectors in his talk, “From Films, to Single Point Detectors to Area Detectors – Fundamentals of Diffraction Geometry”. Prof Mike Glazer (University of Oxford) will explain stereographic projections (and possibly some other useful topics, time permitting!) in a talk entitled “Plotting three-dimensional information in two dimensions.” Prof Bob Eady (University of Liverpool), will then discuss how proteins used to be extracted before modern techniques in “Protein purification before the His-tag era”.

This year, the YCG are co-chairing the “Would you Publish This?” session with the Chemical Crystallography Group in the main meeting. This is an interactive session for which Dr Iain Oswald (University of Strathclyde) is the Keynote speaker. A formal abstract is not required – anyone present can briefly describe one or more structural results that raise the session title question for the audience to discuss – but please contact the session chairs Jorge Sotelo (j.sotelo@ed.ac.uk) or Pascal Parois (pascal.parois@chem.ox.ac.uk) in advance of the meeting (as soon as possible!) if you wish to contribute. The YCG satellite meeting is this year being generously sponsored by the open-access crystallography journal Crystals, for which we are very grateful. Finally, the YCG committee would like to remind the BCA community that anyone (of any age) is welcome to attend the satellite meeting!

In non-meeting news, the YCG vice-chair, Jonathan Brooks-Bartlett (University of Oxford) won his category in the 2015 “I’m a Scientist, Get me out of here” competition. In this competition, school students meet and interact with scientists, who compete for the students’ votes. Jonathan is an excellent communicator and fully deserving of the win, and who also very generously donated his £500 prize to the YCG to be used for YCG-related outreach activities in the future. Other recent outreach activities include a visit from Knowsley School to the University of Liverpool arranged by Dr Sam Horrell and Dr Kate Hammond. A group of 25 children were given a short introduction to what crystallography is and why it is important followed by growing their own lysozyme crystals, making some structural movies and figuring out how DNA bases pair up to form the classic helix shape with the BCA’s MolyMod kit.

We are always happy to hear any feedback or suggestions from any of the members of the YCG, so please contact us on ycg@crystallography.org.uk.

The YCG Committee



Next ACA Meeting

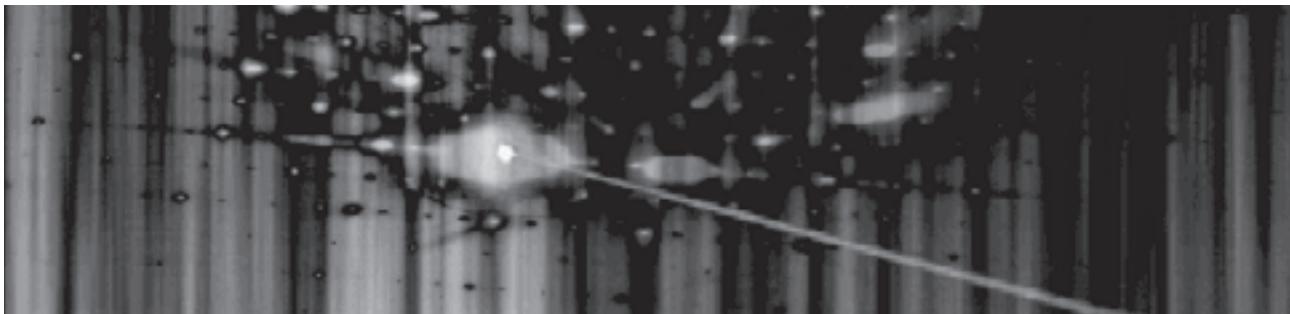
THE 66th Annual Meeting of the American Crystallographic Association (ACA) will be held in Denver, Colorado, July 22 – 26. The transactions symposium will highlight Structural Dynamics across the disciplines represented by the ACA. The rest of the meeting will continue to reflect the wide reach of crystallographic research with sessions on sources, methods, and results. These include Opportunities from new and improved instrumentation, single/multiple crystal, powder and solution methods, and hot structural results. There will be sessions highlighting those results requiring complementary techniques

including cryo-electron microscopy. Invited speakers include this year’s honorees, Jason Benedict (SUNY Buffalo), Axel Brunger (Stanford University), Elspeth Garman (University of Oxford), and Benno Schoenborn (Los Alamos National Laboratory).

The meeting will include a strong educational component for early career scientists with specific talks designed to introduce research areas in addition to presenting results. Related evening sessions include a mixer, career development, and diversity in the laboratory. The conference will end with a closing banquet and the award of poster prizes for the best presentations.

Meeting and Course Announcements

Dynamic Structural Science



THE second workshop on Dynamic Structural Science will be held at Coseners House, Abingdon, 25th- 27th April 2016. The meeting will cover aspects of time-resolved biological structures, molecular photocrystallography, spectroscopy of fast processes, and new science at new radiation sources. More information including on the line up of international speakers can be found on the meeting website <http://www.dynamicstructuralscience.co.uk/>

Next XRF meeting



CALL for papers:

WE are particularly keen to get user and academic talks at this meeting. Please contact any committee member to offer a talk or discuss your contribution. This is a very friendly meeting and is an ideal forum for your first presentation.

Registration Fees:

Early Bird (ends 15th May) £74 or £47 concessions, then £84 or £42 concessions.

A limited number of **FREE STUDENT PLACES** are available at this meeting.

To apply please E-mail **David Beveridge (XRF Chair)** with your name, E-mail address and Institution for details of how to apply for a FREE place. **NOTE:** THE STANDARD REGISTRATION FORM DOES NOT SUPPORT FREE PLACES AND STUDENTS USING IT WILL BE CHARGED CONCESSION FEES.

30th Meeting of the European Crystallographic Association
28 August – 1 September 2016
Congress Center Basel, Switzerland

COME TO BASEL

ABSTRACT SUBMISSION DEADLINE:
April 6th 2016

50 MICROSYMPOSIA
in 5-6 parallel sessions of Biology • Chemistry • Materials • Mineralogy • Physics

ECM-30

<http://ecm30.ecanews.org/ecm2016/home.html>

2016 ICDD Educational Training in XRF & XRD

PRACTICAL XRF & XRD training: live instrumentation, hands-on training and theoretical lectures taught by a highly-talented faculty offering a wide range of application experience.

Practical X-ray Fluorescence Spectrometry

25-29 April 2016

The XRF course covers the basics of X-ray spectra; instrumentation design; methods of qualitative and quantitative analysis; specimen preparation and applications for both wavelength and energy dispersive spectrometry. The course emphasizes quantitative methods; use of automated X-ray spectrometers; review of mathematical matrix correction procedures; and new developments in XRF.

Fundamentals of X-ray Powder Diffraction

16-20 May 2016

The fundamentals clinic covers instrumentation, specimen preparation, data acquisition and qualitative phase analysis through live demonstrations. It also covers hands-on use of personal computers for demonstration of the latest software including data mining with the Powder Diffraction File (PDF) and use of the powder diffractometer: optical arrangement, factors affecting instrumentation profile width, choice and function of divergence slit, calibration and alignment, detectors, and X-ray optics.

Advanced Methods in X-ray Powder Diffraction

23-27 May 2016

The advanced clinic covers factors affecting d-spacings of crystals, as well as factors affecting diffraction-line intensities; structure-sensitive properties (atomic scattering and structure factors), polarization effects, and multiplicity. In addition, the clinic covers specimen-sensitive effects (orientation, particle size), measurement-sensitive effects (use of peak heights and peak areas), and choice of scanning conditions will also be addressed.

Basic Rietveld Refinement & Indexing

26-28 September 2016

Advanced Rietveld Refinement & Indexing

28-30 September 2016

Powder pattern indexing and Rietveld structural refinement techniques are complementary and are often used to completely describe the structure of a material. Successful indexing of a powder pattern is considered strong evidence for phase purity. Indexing is considered a prelude to determining the crystal structure, and permits phase identification by lattice matching techniques. This workshop introduces the theory and formalisms of various indexing methods and structural refinement techniques. One unique aspect of this workshop is the extensive use of computer laboratory problem solving and exercises that teach method development in a hands-on environment.

ICDD Clinic instructors have extensive experience in the field and are deliberately selected from both academia and industry to produce the best of theory and practice. The focus on practical applications, hands-on experience, and intense personal instruction differentiates ICDD clinics from other venues. Each clinic utilizes a team of instructors representing a range of expertise to meet your training needs.

Your registration fee includes all classroom and lab materials, catered lunches as well as morning and afternoon coffee breaks.

Contact: **Eileen Jennings**,
Education Coordinator

Register today at: www.icdd.com/education

E-mail: clinics@icdd.com

Tel: + 610-325-9814

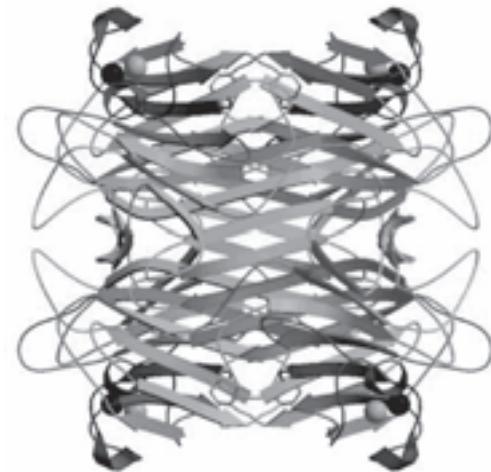


International Year of Pulses

FOLLOWING the peak of excitement in the International Year of Crystallography 2014, the United Nations let us descend gently by declaring 2015 the International Year of Light and Light-based Technologies. After all, X-rays are among the most energetic forms of light. I would argue that crystallographers are among the most energetic researchers using electromagnetic radiation. However, 2016 is the International Year of Pulses (e.g. lentils, beans, peas and chickpeas). What connection could they possibly have with crystallography? There is a connection, actually.

An impressive early achievement of protein crystallography was determination of the structure of concanavalin A (Con A) from jack beans. To be suitable for study back then, a protein had to form very good crystals; and to justify the huge effort required, the results had to have significance to the outside world. This molecule is by no means small: it is a tetramer, each subunit consisting of 237 amino acid residues. Of several publications in the early to mid-1970s, 2CNA in the PDB (Reeve, Becker & Edelman, 1975) reports the structure of ConA to the best resolution (2.00 Å) and includes a wealth of structural information. ConA has remained an interesting subject for research because the high quality of its crystals, allied to advances in technology, has permitted major advances in resolution, culminating in 1NLS, a study to 0.94 Å resolution by Deacon, Gleichmann, Helliwell & Kalb. Following on from this study, Ahmed, Blakeley, Cianci, Hubbard & Helliwell (2007) demonstrated the ability of X-ray diffraction at this resolution, and even with the data truncated to 1.20 Å resolution, to determine the protonation state of aspartic and glutamic acids as well as histidine residues in the molecule. They put forward clear criteria for the reliability of such a determination. Furthermore, they demonstrated the great power of combined neutron and X-ray diffraction to achieve this goal.

There were good medical reasons for all this effort. Jack beans, which are occasionally used as food for humans, and more importantly kidney beans, are toxic because of their content of lectins such as ConA. These lectins bind to sugars, cause various types of cells to agglutinate and can damage the digestive tract. From 1 to 3 hours after eating raw or undercooked beans, victims experience extreme nausea and profuse vomiting. Kidney beans are delicious in chili, but it is imperative that the beans are boiled to destroy the lectins before they are used in the recipe (Wikipedia, 2016). A potential hazard is that a slow cooker does not achieve a sufficiently high temperature. Fortunately, tinned kidney beans have already been heat-treated and are safe to use. Quite apart from its toxicity, ConA is a very useful tool in clinical and biochemical studies. It specifically binds α-D-mannosyl and α-D-glucosyl residues. It was the first commercially available lectin, and it has been used to characterise glycoproteins on the surface of various cells, to purify glycosylated macromolecules by affinity chromatography and to study immune regulation by various immune cells. ConA has been reported to demonstrate potential anti-cancer activity (Li, Xu, Liu & Bao, 2010). It is able to bind to mitochondria, leading to programmed cell death.



Con A (Ahmed, Blakeley, Cianci, Hubbard & Helliwell, 2007)

ConA has been a PDB Molecule of the Month (in the view shown on our cover) because it and favin, another bean protein, are related by circular permutation. This permutation can be envisaged as joining the ends of a protein to make a circle and then snipping the circle in a different place to create new ends. In the ConA / favin case such cutting and pasting is actually performed on the precursor protein. More examples of circular permutation have subsequently been discovered, but the permutation usually occurs in the genome.

Carl Schwalbe

H. U. Ahmed, M. P. Blakeley, M. Cianci, D. W. J. Cruickshank, J. A. Hubbard and J. R. Helliwell (2007) *Acta Cryst. D63*, 906-922.

C.-Y. Li, H.-L. Xu, B. Liu & J.-K. Bao (2010) *Current Molecular Pharmacology*, 3(3): 123-128.

G. N. Reeke Jr., J. W. Becker & G. M. Edelman (1975) *J. Biol. Chem.*, 250, 1535-1547.

https://en.wikipedia.org/wiki/Kidney_beans [Consulted 18 January 2016].



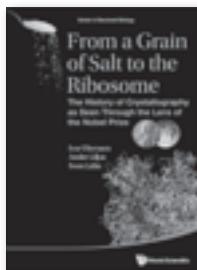
Book Review

Crystallographic Nobel Prizewinners

From a Grain of Salt to the Ribosome: the History of Crystallography as seen through the Lens of the Nobel Prize

Edited by Ivar Olovson, Anders Liljas, and Sven Lidin

Singapore, World Scientific Publishing, 2015. Price GBP98 (Hardcover). ISBN 978-9814623117.



THIS physically heavy book of 519 pages (and some of the copied printing is quite small) surveys the 20 odd crystallographically-related Nobel prizewinners, from the precursor Röntgen, through von Laue and the Braggs to Shechtman (2011) and BK Kobilka (2012). In the UN International Year of Crystallography, the Swedish editors Olovson, Liljas and Lidin have composed typically one- or two- page pleasantly readable biographies with explanations, comments and references for each. In the remaining three-quarters of the volume are reprinted 33 representative articles on the discoveries; at the end is a three-page index.

The Laureates' biographies by Olovson, Liljas and Lidin (the editors don't specify individual responsibility) in chronological sequence of the Award dates are beautifully written, are accompanied by pertinent references and a hint at what the discovery has led to, and occupy about a quarter of the book. They note that Röntgen took out no patents, gave his prize money for research, and both initiated radiography and prepared the way for modern crystallography; the Braggs dispelled the then existing ignorance about the solid state. Rather longer accounts describe the careful discovery of X-rays and the discussions of von Laue (the von dates from 1912) with Sommerfeld and Ewald. Due reference is given to the experiments of Philipp Lenard (who received the Nobel prize in 1905 but as this was for cathode rays his biography is not included). Early Award entries are for the Physics prize but, with the exception of the Award to Crick, Watson and Wilkins for Physiology or Medicine, the later ones are for Chemistry, apart from the one to Brockhouse and Shull.

A colour diagram illustrates how many of the British, German and American macromolecular and other crystallographers are descended from Sir William Henry Bragg and Linus Pauling. Black and white photographs, citations and dates are given for all the scientists. Anders Liljas's Bragg centennial article (though without mention of Forman) in *Acta Cryst* section A of 2013 is reprinted and an account given of the effect on the Braggs and hence on the birth of crystallography of Lars Vegard's communication of von Laue's experiments and theory. The nature of X-rays (WH Bragg was an advocate of the corpuscular theory) is dealt with in the von Laue section. Paul Forman's embellishment of the myth (partly, he surmises to better identify the crystallographic 'clan') about the discovery is presented, together with Ewald's suggestion of artificiality. In the section about the neutron scattering Nobel of 1994, the editors suggest that Shull via diffraction helped answer the question of where atoms are while Brockhouse dealt with what atoms do.

Over the years there is evident a shift towards molecular biology on which neutron diffraction has made a big impact; this shows in many of the more recent discoveries which aid the development of antibiotics. In fact the monograph is one of a Series in Structural Biology. The editors regard the Crick *et al* (1962) DNA model as the 20th century biological finding with richest consequences. Throughout his scientific career, Crick worked most effectively in collaborations. He was one of the scientists who transferred to biology from physics where, during seven years with the Admiralty (merely noted in the book as a Military connection), he had made notable practical contributions to magnetism and electronics. Wilkins had also worked in physics, first in microwaves and radar, then from 1943 on nuclear weapons in the Manhattan Project, an experience that turned him into an ardent opponent of nuclear weapons. Rosalind E Franklin (1920-1958) had studied coal porosity before turning to biophysics. Although never nominated for a Nobel, she came close to determining the DNA structure herself and could have been seriously discussed if she had been alive in 1962. A short biography and a reprinted article are included in the book.

Which have been the most influential crystallographic Nobel Awards?

When large-scale computing could cope with the probabilities, the 1985 Hauptman and Karle Award for tackling the phase problem by Direct Methods, based on atomicity and positivity, transformed crystallography to a process that could be applied across the sciences. In a different way, Pauling's The Nature of the Chemical Bond Award for chemical structure and bonding, rather than one specific discovery, influences a large part of modern chemistry. Awarded the Nobel in 2011 for quasicrystals, Shechtman had a long argument with Pauling who thought twinning was the cause of apparently inconsistent lattice translations. With electron diffraction of some Al alloys with Fe and Mn, Shechtman had observed patterns indicating fivefold or tenfold symmetry in the sample, in conflict with established crystallographic concepts. As a result, the IUCr proposed a new definition: a crystal is any solid with an essentially discrete diffraction diagram.

Although the book title may sound pretentious, the subtitle explains the content exactly. Additional material is given under 'Consequences' and short articles like 'Nature of X-rays' or 'Steps on the Way'. As mentioned, Liljas's article gives the background to the Braggs' discoveries. Olovson, Liljas and Lidin have assembled a valuable compilation of papers and commentaries. The name index is brief but the Awards, accounts and reprinted papers are all in the same date sequence of the prize data.

Derry W Jones,
University of Bradford

Meetings of interest

FURTHER information may be obtained from the websites given. If you have news of any meetings to add to the list, please send them to the Editor, c.h.schwalbe@hotmail.com . Assistance from the IUCr website and the *Journal of Applied Crystallography* is gratefully acknowledged.

2-4 March 2016

CCP-EM Icknield Workshop on Model Building and Refinement for High Resolution EM Maps, Harwell.

<https://eventbooking.stfc.ac.uk/news-events/icknield-workshop-on-model-building-and-refinement-for-high-resolution-em-maps-315>

9-11 March 2016

9th International Workshop on X-ray Radiation Damage to Biological Crystalline Samples, Lund, Sweden.

<http://indico.maxlab.lu.se/event/67/>

13-17 March 2016

251st American Chemical Society National Meeting and Exposition, San Diego, CA, USA.

<http://www.acs.org/content/acs/en/meetings/spring-2016.html>

14-15 March 2016

Spectroscopy Village Analysis, Diamond Light Source.

<http://www.diamond.ac.uk/Home/Events/2016/XASXRF.html>

14-17 March 2016

24th Annual Meeting of the German Crystallographic Society (DGK), Stuttgart, Germany.

<http://www.dgk-conference.de/>

14-18 March 2016

251st American Physical Society March Meeting, Baltimore MD, USA.

<http://www.aps.org/meetings/meeting.cfm?name=MAR16>

29 March – 1 April 2016

TAILOR2016, TAIlored surfaces in Operando conditions: structure and reactivity, Grenoble, France.

<http://www.synchrotron-soleil.fr/portal/page/portal/Accueil/TAILOR-2016/Accueil>

29 March – 29 April 2016

HERCULES 2016 - European School. 26 Years of Neutron & Synchrotron Radiation Science, Fontainebleau, France.

<http://Hercules-school.eu>

30 March – 2 April 2016

2nd International Conference on Image Analysis in Three-dimensional Cryo-EM, Lake Tahoe, CA, USA.

<http://ncmi.bcm.edu/cryoem-software-2016>

31 March – 1 April 2016

International Conference and Exhibition on Materials Chemistry, Valencia, Spain.

<http://materialschemistry.conferenceseries.com/>

4-7 April 2016

BCA Spring Meeting, Nottingham.

<http://www.crystallography.org.uk/bca-spring-meeting-2016/>

10-14 April 2016

Powder Diffraction and Rietveld Refinement School, Durham.

Contact ivana.radosavljevic@durham.ac.uk

11-12 April 2016

Understanding Complex Macromolecular Systems from Sparse Data: The Astbury Conversation, Leeds.

<http://www.astburyconversation.leeds.ac.uk/>

11-15 April 2016

SCTE: 20th International Conference on Solid Compounds of Transition Elements, Zaragoza, Spain.

<http://scte2016.unizar.es/>

12-15 April 2016

ICME 2016, Barcelona, Spain.

<http://congress.cimne.com/icme2016/frontal/default.asp>

19-22 April 2016

Crystallization: Focus on Micro and Nano Crystals and High Throughput Methods, SLAC, Stanford, CA, USA.

http://smb.slac.stanford.edu/news/cryst_focus_on/cryst_focus_on_2016/index.html

24-29 April 2016

RapiData 2016, 18th Annual Course, Stanford, CA, USA.

Contact ana@slac.stanford.edu

24-30 April 2016

ICSM2016: 5th International Conference on Superconductivity and Magnetism, Fethiye / Blue Lagoon, Turkey.

<http://icsm2016.org/>

25-27 April 2016

Workshop on Dynamic Structural Science, Abingdon.

<http://www.dynamicstructuralscience.co.uk/>

25-29 April 2016

Practical X-ray Fluorescence, Newtown Square, PA, USA.

<http://www.icdd.com/education/xrf.htm>

29 April – 1 May 2016

Protein Structure, Dynamics and Function, Providence, RI, USA.

<http://www.brown.edu/conference/sailing-the-protein-seas/>

2-4 May 2016

24th Journées de la Diffusion Neutronique (JDN), Var, France.

<http://jdn-conference.net/>

2-5 May 2016

Integrating X-ray crystallography and scattering with electron microscopy, Oeiras (NOVA ITQB), Portugal.

<http://www.itqb.unl.pt/CombStruct2016>

2-6 May 2016

2016 E-MRS Spring Meeting and Exhibit, Lille, France.

<http://www.european-mrs.com/meetings/2016-spring-meeting>

16-20 May 2016

7th Workshop on Neutron Scattering Applications in Structural Biology, Oak Ridge, TN, USA.

<https://conference.sns.gov/event/15/>

16-20 May 2016

Fundamentals of X-ray Powder Diffraction, Newtown Square, PA, USA.

<http://www.icdd.com/education/xrd.htm>

19-21 May 2016

6th Meeting on X-ray and Other Techniques in Investigations of the Objects of Cultural Heritage, Krakow, Poland.

<http://www.biurokarter.chemia.uj.edu.pl/conf/x-ray16>

21-26 May 2016

Structural characterization of macromolecular complexes, Grenoble, France.

<http://events.embo.org/coming-soon/index.php?EventID=pc16-23>

22-26 May 2016

Chromatin Structure & Function (GRC), Les Diablerets, Switzerland.

<http://www.grc.org/programs.aspx?id=11783>

23-27 May 2016

Advanced Methods in X-ray Powder Diffraction, Newtown Square, PA, USA.

<http://www.icdd.com/education/xrd.htm>

24-27 May 2016

Introduction to ISIS and Diamond facilities for CDT students 2016, Rutherford Appleton Laboratory.

<http://www.diamond.ac.uk/Home/Events/2016/CDT-Workshop.html>

25-29 May 2016

Macromolecular Crystallography School 2016 (MCS2016), Madrid, Spain.

<http://www.xtal.iqfr.csic.es/MCS2016/>

27 May – 1 June 2016

Molecular basis of human diseases, Spetses, Greece.

http://www.eie.gr/nhrf/institutes/ibrb/spetses-2016/welcome_message.html

27 May – 5 June 2016

High-Pressure Crystallography: Status Artis and Emerging Opportunities. 49th Erice Course, Erice, Sicily, Italy.

<http://www.crystalerice.org/2016>

29 May – 1 June 2016

Microtubules: From Atoms to Complex Systems, Heidelberg, Germany.

<http://www.embo-embl-symposia.org/symposia/2016/EES16-04/index.html>

29 May – 3 June 2016

ISC Granada 2016. 5th International School on Crystallization, Granada, Spain.

<http://www.iscgranada.org/>

29 May – 4 June 2016

3rd International Summer School of Crystallography (ISSC16), Hamburg, Germany.

<http://conferences.cfel.de/issc16>

30 May – 4 June 2016

Computational analysis of protein-protein interactions: Sequences, networks and diseases, Budapest, Hungary.

<http://events.embo.org/16-protein-protein/>

5-9 June 2016

11th USPEX Workshop on Evolutionary and Interpretation Methods for Discovering the Structures and Rationalizing the Properties of Crystalline Surface and Nanoparticle Materials, Lake Como, Italy.

5-10 June 2016

Bioinspired Materials. Gordon Research Conference, Les Diablerets, Switzerland.

<http://www.grc.org/programs.aspx?id=15059>

6-9 June 2016

IWPCPS-17: International Workshop for Physical Characterization of Pharmaceutical Solids, Winter Park, FL, USA.

<http://www.assainternational.com/workshops/iwpcps-17/>

6-10 June 2016

ED-XPD Workshop – Combining Electron and X-ray Powder Diffraction Techniques for Structural Characterization, Stockholm, Sweden.

7-10 June 2016

Biophysics in Drug Discovery 2016. 3rd NovAliX Conference, Strasbourg, France.

<http://www.novalix-conferences.org>

7-10 June 2016

COHERENCE2016. International Workshop on Phase Retrieval and Coherent Scattering, Saint Malo, France.

<http://www.synchrotron-soleil.fr/portal/page/portal/Soleil/ToutesActualites/Workshops/2016/COHERENCE-2016>

10-13 June 2016

13th TOPAS User's Meeting, Bari, Italy.

<http://www.bruker.com/events/users-meetings/x-ray-diffraction-and-elemental-analysis/topas-users-meeting.html>

12-15 June 2016

15th European Powder Diffraction Conference (EPDIC15), Bari, Italy.

<http://www.ba.ic.cnr.it/epdic15/>

12-15 June 2016

RNA structure meets function. EMBO Workshop, Stockholm, Sweden.

<http://events.embo.org/16-rna/>

12-15 June 2016

The biochemistry and chemistry of biocatalysis: From understanding to design, Oulu, Finland.

<http://events.embo.org/16-biocatalysis/>

15 June 2016

BCA Industrial Group XRF Meeting, Leicester.

<https://sites.google.com/site/bcaxrf/>

19-22 June 2016

74th Device Research Conference (DRC 2016), Newark, DE, USA.

<http://www.mrs.org/drc-2016/>

19-24 June 2016

European Conference on X-Ray Spectrometry EXRS2016, Gothenburg, Sweden.

<http://www.exrs2016.se>

22-24 June 2016

58th Electronic Materials Conference, Newark, DE, USA.

<http://www.mrs.org/58th-emc/>

26 June – 1 July 2016

7th European Charge Density Meeting (ECDM7), Warsaw, Poland.

<http://ecd7.chem.uw.edu.pl/>

27 June – 2 July 2016

Advanced Methods in Macromolecular Crystallization VII, Nove Hrady, Czech Republic.

<http://www.crystallography.fr/mathcryst/antwerp2016.php>

27 June – 3 July 2016

International School on Fundamental Crystallography with Applications to Electron Crystallography, Antwerp, Belgium.

<http://www.crystallography.fr/mathcryst/antwerp2016.php>

2-7 July 2016

ICCBM-16. 16th International Conference on the Crystallization of Biological Macromolecules, Prague, Czech Republic.

<http://www.iccbm16.org/>

3-8 July 2016

6th international conference on NANOfstructures and nanomaterials SElf-Assembly (NANOSEA), Giardini Naxos, Italy.

<http://www.nanosea2016.imm.cnr.it>

4-8 July 2016

3rd International School on Aperiodic Crystals, Antwerp, Belgium.

<https://www.uantwerpen.be/en/summer-schools/aperiodic-crystals/>

4-9 July 2016

Integrative modelling of biomolecular interactions. EMBO Practical Course, Barcelona, Spain.

<http://events.embo.org/16-biomol-interact/>

6-8 July 2016

British Biophysical Society Biennial Conference, Liverpool.

www.bbs2016.co.uk

6-10 July 2016

Ribosome Structure and Function, Strasbourg, France.

<http://events.embo.org/16-ribo/>

10-14 July 2016

American Conference on Neutron Scattering, Long Beach, CA, USA.

<http://www.mrs.org/acns-2016/>

10-15 July 2016

18th International Conference on Metal Organic Vapor Phase Epitaxy (ICMOVPE-XVIII), San Diego, CA, USA.

<http://www.mrs.org/icmovpe-xviii/>

10-15 July 2016

FASEB Summer Research Conference on Post-transcriptional control of gene expression: Mechanisms of RNA decay. EMBO Keynote Lecture, Lisbon, Portugal.

<http://www.faseb.org/SRC-Microsite/mRNA/Home.aspx>

16-19 July 2016

The Protein Society Conference. The 30th Anniversary Symposium of The Protein Society, Baltimore, MD, USA.

<http://www.proteinsociety.org/meetings/symposium/>

18-22 July 2016

SymFest'16. Symmetry Festival, Vienna, Austria.

<http://festival.symmetry.hu/>

21-25 July 2016

12th International Congress of Cell Biology, Prague, Czech Republic.

<http://iccb2016.org/>

22-26 July 2016

American Crystallographic Association Annual Meeting, Denver, CO, USA.

<http://www.americaltassn.org/content/pages/main-annual-meetings>

24-29 July 2016

Virus Structure and Assembly, Steamboat Springs, CO, USA.

<http://www.faseb.org/SRC-Microsite/VStruc/Home.aspx>

31 July - 5 August 2016

Machines on Genes IV. 80th Harden Conference, Macclesfield, Cheshire.

<http://www.biochemistry.org/Events/tbid/379/Page/2/MeetingNo/80HDN/view/Conference/Default.aspx>

1-5 August 2016

Denver X-ray Conference. 65th Annual Conference on Applications of X-ray Analysis, Rosemont, IL, USA.

<http://www.dxcicdd.com/>

7-12 August 2016

18th International Conference on Crystal Growth and Epitaxy ICCGE-18, Nagoya, Japan.

<http://www.iccge18.jp/>

15-19 August 2016

X-Ray Microscopy Conference 2016 (XRM2016), Oxford.

<http://www.xrm2016.com/>

21-24 August 2016

12th International Conference on Biology and Synchrotron Radiation (BSR), SLAC National Accelerator Laboratory, CA, USA.

<https://conf-slac.stanford.edu/bsr-2016>

22-23 August 2016

International Conference on Structural Biology, New Orleans, LA, USA.

<http://structuralbiology.conferenceseries.com/events-list/hybrid-approches-for-structure-prediction>

22-26 August 2016

Joint European Magnetic Symposia (JEMS), Glasgow.

<http://jems2016.iopconfs.org>

22-26 August 2016

Powder Diffraction School. Modern Synchrotron Methods, Villigen, Switzerland.

<https://indico.psi.ch/conferenceDisplay.py?confId=2592>

23-26 August 2016

International School on Charge and Spin Density: From Experimental Determination to Interpretation, Nancy, France.

<http://crm2.univ-lorraine.fr/lab/education/congres/ecm30-congress-satellite-school/>

28 August – 1 September 2016

European Crystallographic Association Meeting, Basel, Switzerland.

<http://ecm30.ecanews.org/ecm2016/home.html>

4-8 September 2016

XTOP 2016 – 13th Biennial Conference on High-Resolution X-Ray Diffraction and Imaging, Brno, Czech Republic.

<http://xtop2016.sci.muni.cz/>

4-9 September 2016

The 54th European High Pressure Research Group (EHPRG) International Meeting on High Pressure Science and Technology, Bayreuth, Germany.

<http://www.ehprg2016.org/>

4-9 September 2016

The 16th International Conference on Liquid and Amorphous Metals (LAM-16), Bonn – Bad Godesberg, Germany.

<https://dlr-mp.meetingmasters.de/LAM16>

5-8 September 2016

Quasielastic neutron scattering QENS 2016, Berlin, Germany.

http://www.helmholtz-berlin.de/events/qens-2016/index_de.html

7-10 September 2016

Actin in action: From molecules to cellular functions. EMBO | EMBL Symposium, Heidelberg, Germany.

<http://www.embo-embl-symposia.org/symposia/2016/EES16-06/index.html>

8-9 September 2016

WINS2016: Workshop on Inelastic Neutron Spectrometers, Berlin, Germany.

http://www.helmholtz-berlin.de/events/qens-2016/wins-2016/index_de.html

11-15 September 2016

5th International Conference on Metal-Organic Frameworks & Open Framework Compounds (MOF 2016), Long Beach, CA, USA.

<http://www.mrs.org/mof-2016/>

11-16 September 2016

MEDSI2016. Mechanical Engineering Design of Synchrotron Radiation Equipment and Instrumentation, Barcelona, Spain.

<https://indico.cells.es/indico/event/42/>

12-20 September 2016

Protein expression, purification, and characterization (PEPC10), Hamburg, Germany.

<http://events.embo.org/coming-soon/index.php?EventID=pc16-22>

25 September – 2 October 2016

3rd European Crystallography School (ECS3), Bol, Croatia.

<http://3redeuropeancrystallographyschool.weebly.com/>

29 September – 1 October 2016

19th Heart of Europe Biocrystallography Meeting, Warberg, Germany.

http://www.helmholtz-hzi.de/de/aktuelles/veranstaltungen/hec_19_meeting/overview/

2-7 October 2016

International Workshop on Nitride Semiconductors (IWN 2016), Orlando, FL, USA.

<http://www.mrs.org/iwn-2016>

2-7 October 2016

Retinal proteins. EMBO Conference, Potsdam, Germany.

<http://events.embo.org/16-retinal-proteins/>

17-19 October 2016

International Conference on Applied Crystallography, Houston, TX, USA.

17-24 October 2016

Solution scattering from biological macromolecules. EMBO Practical Course, Hamburg, Germany.

<http://events.embo.org/coming-soon/index.php?EventID=pc16-20>

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650°C
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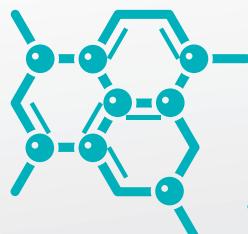
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